BENEMÉRITA UNIVERSIDAD AUTÓNOMA DE PUEBLA

INSTITUTO DE FÍSICA
"Luis Rivera Terrazas"

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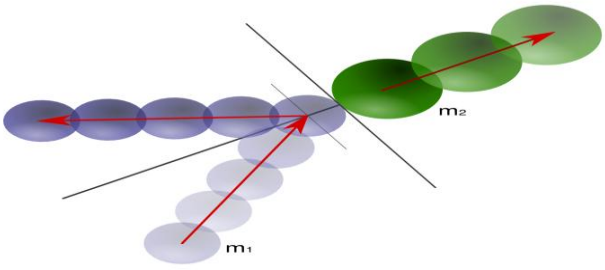
"DR. JESUS REYES CORONA"



"Electronic and magnetic properties of graphene nanoflakes"

Dr. Romeo de Coss
Department of Applied Physics,
Cinvestav-Mérida, México.

The electronic structure of graphene corresponds to a semi-metal with p-electrons at Fermi level, which are responsible of the unique electronic properties for this material. Graphene nanostructures show an energy gap resulting of the finite size, and are of current interest because of the potential applications in electronic and optoelectronic devices. Thus, we discuss some recent progress in the synthesis of graphene nanoflakes obtained from the reaction of polyaromatic hydrocarbons. In this talk, we are presenting ab-initio results for the electronic and magnetic properties of graphene nanoflakes of different sizes and shapes. The optical gap of hexagonal zig-zag nanoflakes is obtained from the ab-initio calculculations of the quasiparticle gap and the exitonic binding energy estimaed from an effective mass model. We found that the energy gap of graphene nanoflakes decreases with size following an exponential scaling rule. Secondly, the problem of determining the magnetic moment of graphene nanoflakes with single-vacancy defects is addressed. Using the Fixed Spin Moment method, the ground state spin multiplicity and the spin magnetic distribution was obtained. We found that the ground state multiplicity is triplet, corresponding to a spin magnetic moment of 2 μ_B. From the analysis of the orbital spin distribution we found that the spin-polarized is equally distributed in the sp^2 and p_z orbitals. Work supported by Conacyt-México under Grant No. 83604.

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17:00 Hrs.